Multiscale Assembly of Epitaxial Semiconductor Heterostructures

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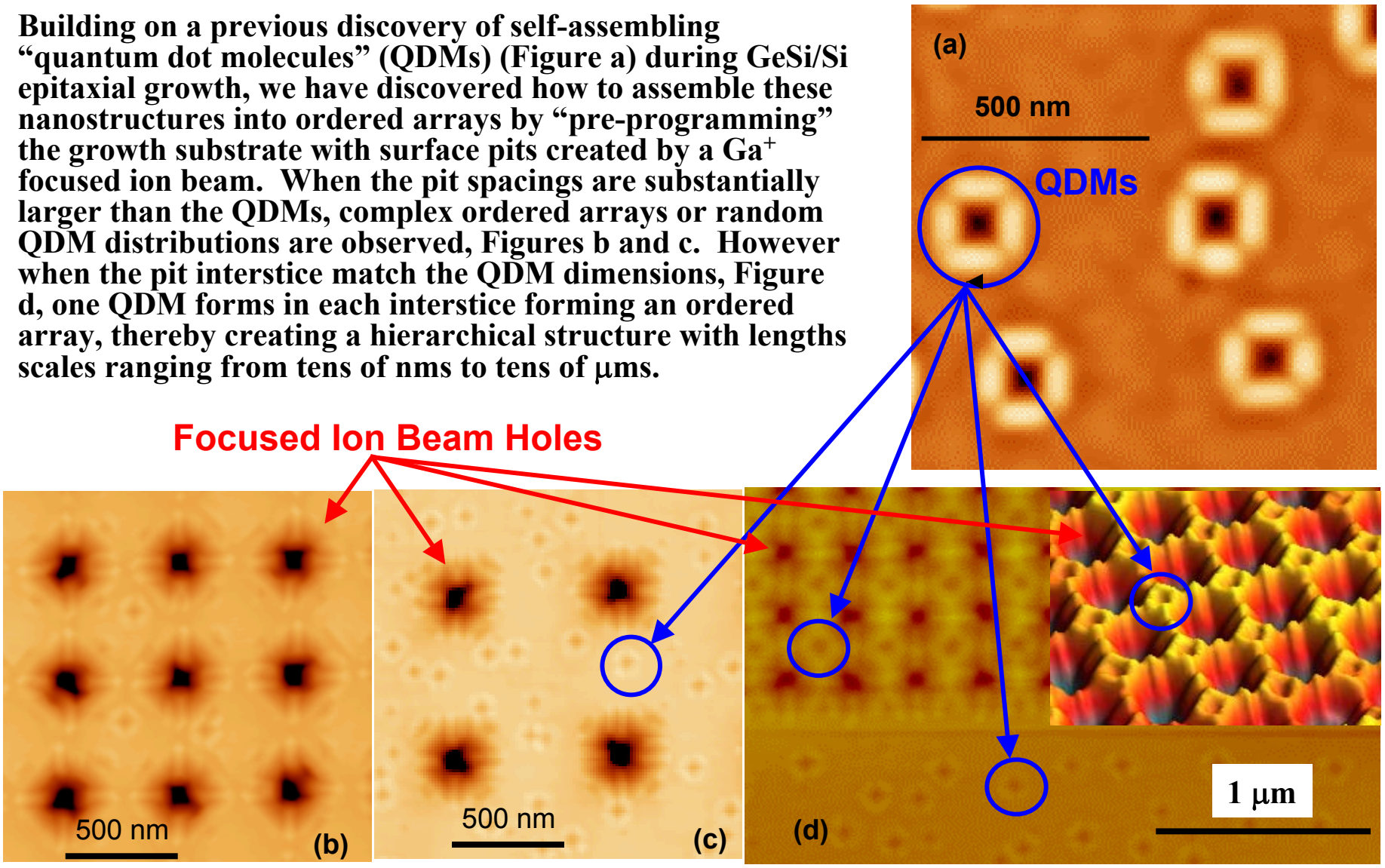
Focused Research Group DMR – 0075116

Building on a previous discovery of self-assembling "quantum dot molecules" (QDMs) (Figure a) during GeSi/Si epitaxial growth, we have discovered how to assemble these nanostructures into ordered arrays by "pre-programming" the growth substrate with surface pits created by a Ga^+ focused ion beam. When the pit spacings are substantially larger than the QDMs, complex ordered arrays or random QDM distributions are observed, Figures b and c. However when the pit interstice match the QDM dimensions, Figure d, one QDM forms in each interstice forming an ordered array, thereby creating a hierarchical structure with lengths scales ranging from tens of nms to tens of μms.



Samples are grown at Sandia by MBE; All images are AFM tapping mode; Note that in (d) QDM in unpatterned regions remains random; Patterned Structures are Si0.7Ge0.3, 535C, 0.9A/s, 200A film on 360A Si buffer; Ex-situ focused ion beam patterning is done with a 30 keV gallium beam.

Motivation – heteroepitaxy of lattice-mismatched semiconductor materials can produce self-assembling islands or "quantum dots (QDs)" of the deposited material. The dimensions of these QDs – typically of order tens of nanometers – make them candidates for use as individual electronic elements in exploratory nanoelectronic architectures. However, this self-assembly process is inherently random. We are seeking ways to realize control of the self-assembly processes such that the QDs can be organized into configurations of potential practical use.

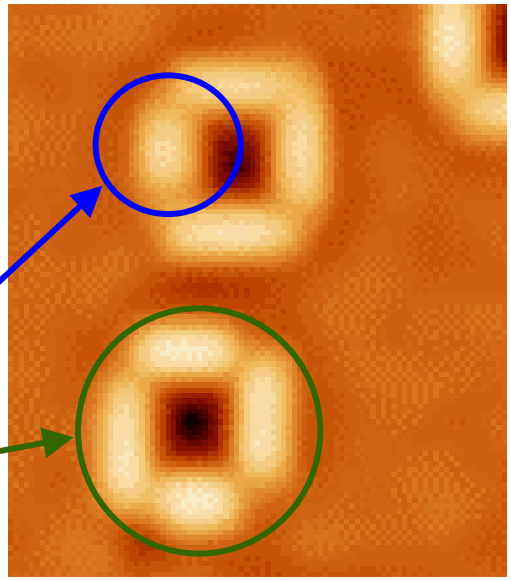
Discovery 1 – we have previously discovered under this program funding a new self-assembling nanostructure in the GeSi/Si system: the quantum dot molecule (QDM) This comprise a multi-component self-assembling structure of four-fold {510}-facetted islands organizing around {510}-facetted strain-relieving pits. These structures form under a range of epitaxial growth conditions where the surface atom mobility during growth is sufficient to allow coalescence into the QDMs, but is insufficient to allow the less complex equilibrium structures that form in this system. We thus have an entirely new self-assembling unit or "building block" at the nanoscale, with overall dimensions of order 100 – 400 nm depending upon the strain in the system. We have shown that these structures self-limit in terms of both shape (defined by {510} facets) and size (which arrests when the four-fold islands close around the pit perimeter). Thus we we can generate enormous quantities (c. 10^9 cm^{-2}) of a building block that has direct relevance to potential nanoelectronic architectures such as QCA (Quantum Cellular Automata) cells.

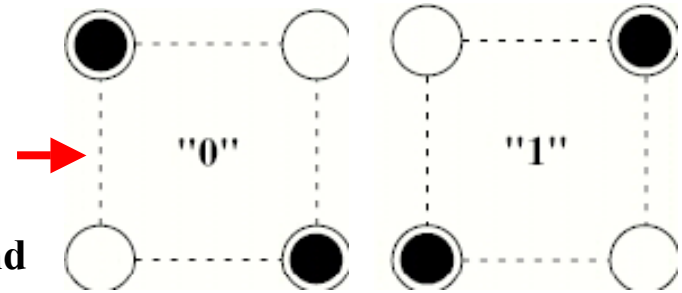
Discovery 2 – on an unmodified Si(100) surface the QDMs form randomly, although each QDM has exquisite organization within itself. Our latest result is to use focused ion beam topographical patterning of the growth surface prior to deposition, to create interstices upon which the QDMs are forced to grow. The evolution of those FIB-induced features is itself complex and fascinating – during both Si and GeSi epitaxial growth, the holes expel material and enlarge with formation of {311} facets in the initial Si buffer layer, followed by formation of {510} facets in the GeSi layer. Thus the final diameter (i.e. at the growth surface) of the holes and the interstices between them depends upon the initial hole dimensions, their spacings, and the deposited film thicknesses. We have successfully identified conditions which enable matching of interstice dimensions to the QDMs, thus enabling ordered arrays of QDMs to be fabricated.

Significance. **This work demonstrates the capability to combine natural self-assembly processes –where nature provides enormous quantities of well-defined nanoscale building blocks – with external lithographic guiding of the self-assembly process. This provides paths for assembly of nano-objects into controlled large scale systems. In the present case the system is created at several hierarchical length scales. The smallest length scale corresponds to individual components of the Quantum Molecule at tens of nms. The next length scale is that of the QDM, at hundreds of nms. The largest length scale is that of the topographic forcing function, with tens of microns demonstrated, and macroscopic lengths scales in principle accessible.**

Broader Impacts

- **New structures in epitaxial materials – QDM discovered under this focused research group.**
  - **Four-fold {510}-facetted islands self-assemble around {510}-facetted strain-relieving pits**
  - **Size and shape of QDMs self-limit at dimensions controlled by system strain**
- **Combining natural self-assembly with lithographic guiding – a route to higher definition structuers for the semiconductor industry?**
  - **Smallest length scale corresponds to individual components of the Quantum Dot Molecule, c. 50 nm**
  - **Next length scale is that of mature QDM, c. 200 nm**
  - **Largest length scale is of topographic pattern controlling QDM formation - tens of microns demonstrated.**
- **Potential applications to new nanoelectronic architectures**
  - **Many in the semiconductor industry believe a key route to further miniaturization is to couple self-assembly to local lithographic definition**
  - **Specific applications to Quantum Cellular Automata (QCAs)**
- **Highly effective collaboration between university (UVa) and government laboratory (Sandia)**
  - **UVa graduate student Jennifer Gray has spent multiple trips of several weeks working at Sandia**
  - **Access to facilities of new DOE nanocenter ar Sandia (CINT)**





QCA: Electronic charges in quadruplet dots form bistable states due to charge repulsion, mimicing binary states of digital logic